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Geometric means

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Abstract

We propose a definition for geometric mean of k positive (semi) definite matrices. We show that our definition is the only one in the literature that has the properties that one would expect from a geometric mean, and that our geometric mean generalizes many inequalities satisfied by the geometric mean of two positive semidefinite matrices. We prove some new properties of the geometric mean of two matrices, and give some simple computational formulae related to them for 2×2 matrices.

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1. Introduction

The geometric mean of two positive semidefinite matrices arises naturally in several areas, and it has many of the properties of the geometric mean of two positive scalars. Researchers have tried to define a geometric mean on three or more positive definite matrices, but there is still no satisfactory definition. In this paper we present a

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definition of the geometric mean of three or more positive semidefinite matrices and show that it has many properties one would want of a geometric mean. We compare our definition with those proposed by other researchers.

Let us consider first what properties should be required for a reasonable geometric mean $G(A, B, C)$ of three positive definite matrices A, B, C. It is clear what the corresponding conditions would be for k matrices for $k > 3$.

P1 Consistency with scalars. If A, B, C commute then $G(A, B, C) = (ABC)^{1/3}$.
P1′ This implies $G(A, A, A) = A$.
P2 Joint homogeneity. $G(\alpha A, \beta B, \gamma C) = (\alpha\beta\gamma)^{1/3} G(A, B, C) \qquad (\alpha, \beta, \gamma > 0)$.
P2′ This implies $\quad G(\alpha A, \alpha B, \alpha C) = \alpha G(A, B, C) \qquad (\alpha > 0)$.
P3 Permutation invariance. For any permutation $\pi(A, B, C)$ of (A, B, C)

$$G(A, B, C) = G(\pi(A, B, C)).$$

P4 Monotonicity. The map $(A, B, C) \longmapsto G(A, B, C)$ is monotone, i.e., if $A \geqslant A_0$, $B \geqslant B_0$, and $C \geqslant C_0$, then $G(A, B, C) \geqslant G(A_0, B_0, C_0)$ in the positive semidefinite ordering.
P5 Continuity from above. If $\{A_n\}, \{B_n\}, \{C_n\}$ are monotonic decreasing sequences (in the positive semidefinite ordering) converging to A, B, C, respectively, then $\{G(A_n, B_n, C_n)\}$ converges to $G(A, B, C)$.
P6 Congruence invariance.

$$G(S^*AS, S^*BS, S^*CS) = S^*G(A, B, C)S \quad \text{for any invertible } S.$$

P7 Joint concavity. The map $(A, B, C) \longmapsto G(A, B, C)$ is *jointly concave*:

$$\begin{aligned} &G(\lambda A_1 + (1-\lambda)A_2, \lambda B_1 + (1-\lambda)B_2, \lambda C_1 + (1-\lambda)C_2) \\ &\quad \geqslant \lambda G(A_1, B_1, C_1) + (1-\lambda)G(A_2, B_2, C_2) \qquad (0 < \lambda < 1). \end{aligned}$$

P8 Self-duality. $G(A, B, C) = G(A^{-1}, B^{-1}, C^{-1})^{-1}$.
P9 Determinant identity. $\det G(A, B, C) = (\det A \cdot \det B \cdot \det C)^{1/3}$.

These properties are desirable, and perhaps we can add more desirable properties to the list, but any geometric mean should satisfy properties P1–P6 at a bare minimum. These properties quickly imply other properties, as we now discuss.

Notice that P2 and P4 imply P5. In fact, denote by $\rho(X)$ the spectral radius of X. By P4 we will have

$$\begin{aligned} &\rho(A_n^{-1}A)^{-1}A \leqslant A_n \leqslant \rho(A^{-1}A_n)A, \\ &\rho(B_n^{-1}B)^{-1}B \leqslant B_n \leqslant \rho(B^{-1}B_n)B, \\ &\rho(C_n^{-1}C)^{-1}C \leqslant C_n \leqslant \rho(C^{-1}C_n)C. \end{aligned}$$

Now, setting $G = G(A, B, C)$ and $G_n = G(A_n, B_n, C_n)$, condition P2 gives

$$\begin{aligned} &[\rho(A_n^{-1}A)\rho(B_n^{-1}B)\rho(C_n^{-1}C)]^{-1/3}G \\ &\quad \leqslant G_n \leqslant [\rho(A^{-1}A_n)\rho(B^{-1}B_n)\rho(C^{-1}C_n)]^{1/3}G. \end{aligned} \tag{1.1}$$

Thus, if $(A_n, B_n, C_n) \longrightarrow (A, B, C)$ then $G(A_n, B_n, C_n) \longrightarrow G(A, B, C)$.

Notice that invertibility is essential in the above proof.

By P1, P3, P7, and P8, we have

P10 The arithmetic–geometric–harmonic mean inequality.

$$\frac{A+B+C}{3} \geqslant G(A, B, C) \geqslant \left(\frac{A^{-1}+B^{-1}+C^{-1}}{3}\right)^{-1}.$$

If we partition all matrices conformally:

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22} \end{pmatrix}$$

and define the *pinching operator* Φ by

$$\Phi(A) = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix},$$

then

$$\Phi(A) = (A + S^*AS)/2 \quad \text{with } S = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.$$

Now, concavity, homogeneity and congruence invariance, yield

$$\Phi(G(A, B, C)) \leqslant G(\Phi(A), \Phi(B), \Phi(C)). \tag{1.2}$$

Once a geometric mean for three positive definite matrices is defined so as to satisfy P1–P6, by monotonicity we can uniquely extend the definition of $G(A, B, C)$ for every triple of positive semidefinite matrices (A, B, C) by setting

$$G(A, B, C) = \lim_{\epsilon \downarrow 0} G(A + \epsilon I, B + \epsilon I, C + \epsilon I).$$

Then it is immediate to see that by P5 for positive definite A, B, C the new definition coincides with the original one for positive definite A, B, C and that the extended geometric mean satisfies P1–P4 and P6. Since it is easy to see that for positive semidefinite A, B, C

$$G(A, B, C) = \inf\{G(\tilde{A}, \tilde{B}, \tilde{C}) : \tilde{A} > A, \tilde{B} > B, \tilde{C} > C\},$$

P5 is valid for this extended geometric mean. If the original geometric mean satisfies P7, so does the extended one.

We can derive a stronger form of P6 with help of P4 and P5:

P6′ $G(S^*AS, S^*BS, S^*CS) \geqslant S^*G(A, B, C)S$ for all S.

In fact, if S is not invertible, let $S_\epsilon = (1-\epsilon)S + \epsilon I$ for $0 < \epsilon < 1$. Then by P6

$$G(S_\epsilon^*AS_\epsilon, S_\epsilon^*BS_\epsilon, S_\epsilon^*CS_\epsilon) = S_\epsilon^*G(A, B, C)S_\epsilon.$$

The right-hand side converges to $S^*G(A, B, C)S$ as $\epsilon \to 0$. Since by the operator convexity of the square function, for any $X \geqslant 0$

$$(1-\epsilon)S^*XS+\epsilon X \geqslant ((1-\epsilon)S^*+\epsilon I)X((1-\epsilon)S+\epsilon I)$$

and

$$S^*XS+\epsilon X \geqslant (1-\epsilon)S^*XS+\epsilon X,$$

by P4 (monotonicity) we have

$$G(S^*AS+\epsilon A, S^*BS+\epsilon B, S^*CS+\epsilon C) \geqslant G(S_\epsilon^*AG_\epsilon, S_\epsilon^*BG_\epsilon, S_\epsilon^*CG_\epsilon).$$

Since $S^*XS+\epsilon X$ converges downward to S^*XS as $\epsilon \downarrow 0$, by P5 (continuity from above) we conclude the inequality.

Our paper is organized as follows. In Section 2, we present some properties for the geometric mean of two matrices, which will be useful when we define our geometric means for three or more matrices, and when we compare our definition with those proposed by others. In Section 3, we present our definition of geometric means for three or more matrices, and show that it has all the desirable properties P1–P9. We then compare our definition with those of others in Sections 4 and 5. In Section 6, we present some formulae for different geometric means of 2×2 matrices. The formulae may be helpful for future study of the topic.

2. The geometric mean of two matrices

Conditions P1 and P6 are sufficient to determine the geometric mean of two positive definite matrices A and B. There is a non-singular matrix S that simultaneously diagonalizes A and B by congruence:

$$A = S^*D_AS \quad \text{and} \quad B = S^*D_BS \tag{2.1}$$

for some diagonal matrices D_A and D_B. For example, one can choose $S = U^*A^{1/2}$ where U is unitary such that $U^*A^{-1/2}BA^{-1/2}U$ is a diagonal matrix. Since the diagonal matrices D_A and D_B commute we have

$$\begin{aligned} G(A, B) &= G(S^*D_AS, S^*D_BS) \\ &= S^*G(D_A, D_B)S \\ &= S^*(D_AD_B)^{1/2}S. \end{aligned}$$

One can show that the value of $S^*(D_AD_B)^{1/2}S$ is independent of the choice of the matrix S. Thus we can compute $G(A, B)$ numerically.

Actually there are many equivalent definitions of the geometric mean of two positive definite matrices A and B. Researchers have tried to use these conditions to define geometric means of three or more matrices (see [2,4,7,9] and their references, and see also Sections 4 and 5).

D1 $G(A, B) = S^*(D_AD_B)^{1/2}S$, where S is any invertible matrix that simultaneously diagonalizes A and B by congruence as in (2.1).

D2 $G(A, B)$ is the solution to the extremal problem

$$\max\left\{X \geqslant 0 : \begin{pmatrix} A & X \\ X & B \end{pmatrix} \geqslant 0\right\}.$$

D3 $G(A, B) = A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2}$
In fact, one can use the fact that a function of a matrix is a polynomial in the matrix to show that $G(A, B) = A^{1-p}(A^{p-1}BA^p)^{1/2}A^p$, for any $p \in \mathbb{R}$, but there seems no advantage in choosing $p \neq 1/2$.

D4 $G(A, B) = A^{1/2}UB^{1/2}$, where U is any unitary matrix that makes the right-hand side positive definite. For example, we can let $U = (A^{-1/2}BA^{-1/2})^{1/2} A^{1/2}B^{-1/2}$ so that $A^{1/2}UB^{1/2} = A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2}$. Note that even when the choice of U is not unique, the value of $A^{1/2}UB^{1/2}$ is unique.
This definition has rarely been stated, but it will be useful in this paper.

D5 $G(A, B)$ is the value of the definite integral

$$\frac{1}{\Gamma(1/2)^2}\int_0^1 \{\lambda B^{-1} + (1-\lambda)A^{-1}\}^{-1}\{\lambda(1-\lambda)\}^{-1/2}\,\mathrm{d}\lambda.$$

This is actually the special case for $k = 2$ of a geometric mean proposed by Kosaki [7] and modified by Kubo and Hiai.

To conclude this section we present some new computational results for $G(A, B)$.

Proposition 2.1. *Let* $A, B > 0$ *be* 2×2 *and such that* $\det(A) = \det(B) = 1$. *Then*

$$G(A, B) = \frac{A + B}{\sqrt{\det(A + B)}}. \tag{2.2}$$

Proof. Let S be a matrix with $\det(S) = 1$, that simultaneously diagonalizes A and B by congruence. Then since A, B, and S all have determinant equal to 1 we have:

$$A = S^*\begin{pmatrix} a & 0 \\ 0 & a^{-1} \end{pmatrix} S, \quad \text{and} \quad B = S^*\begin{pmatrix} b & 0 \\ 0 & b^{-1} \end{pmatrix} S.$$

$$\begin{aligned} G(A, B) &= S^*\begin{pmatrix} \sqrt{ab} & 0 \\ 0 & \frac{1}{\sqrt{ab}} \end{pmatrix} S \\ &= \frac{1}{\sqrt{(a+b)(a^{-1}+b^{-1})}} S^*\begin{pmatrix} a+b & 0 \\ 0 & a^{-1}+b^{-1} \end{pmatrix} S \\ &= \frac{A+B}{\sqrt{\det(A+B)}}. \qquad \square \end{aligned}$$

Corollary 2.2. *Let* $A, B > 0$ *be* 2×2. *Let* $s = \sqrt{\det(A)}$, $t = \sqrt{\det(B)}$. *Then*

$$G(A, B) = \frac{\sqrt{st}}{\sqrt{\det(s^{-1}A + t^{-1}B)}}(s^{-1}A + t^{-1}B); \tag{2.3}$$

in particular,

$$A^{1/2} = G(A, I) = \frac{\sqrt{s}}{\sqrt{\det(s^{-1}A + I)}}(s^{-1}A + I). \tag{2.4}$$

One can prove (2.4) directly using the arguments in the proof of Proposition 2.1. More generally, for any continuous function $f : \mathbb{R}_+ \to \mathbb{R}$, if A is a 2×2 positive definite matrix with eigenvalues $a, b \in (0, \infty)$, then $f(A) = rA + sI$ with

$$r = \frac{f(a) - f(b)}{a - b} \quad \text{and} \quad s = \frac{af(b) - bf(a)}{a - b}.$$

Since

$$a = \frac{1}{2}\left\{\mathrm{tr}A + \sqrt{(\mathrm{tr}A)^2 - 4\det(A)}\right\}, \quad b = \frac{1}{2}\left\{\mathrm{tr}A - \sqrt{(\mathrm{tr}A)^2 - 4\det(A)}\right\}$$

and $\mathrm{tr}A = \sqrt{\det(A)}[\det\left(I + A/\sqrt{\det(A)}\right) - 2]$, one can express $f(A) = r(A)A + s(A)I$ for suitable functions $r(A)$ and $s(A)$ that only involve $\det(A)$ and $\det(I + A/\sqrt{\det(A)})$.

3. Geometric means of three or more matrices

Recall that $\rho(X)$ denotes the spectral radius of X. We will use a limiting process to define a new geometric mean. In proving convergence we will use the following multiplicative metric on the space of pairs of positive definite matrices:

$$R(A, B) = \max\{\rho(A^{-1}B), \rho(B^{-1}A)\}. \tag{3.1}$$

Note that $\rho(A^{-1}B) = \rho(A^{-1/2}BA^{-1/2}) = \rho(B^{1/2}A^{-1}B^{1/2})$. The metric $R(\cdot, \cdot)$ has many nice properties, for example, in the scalar case, we have

$$R(a, b) = \max\{a/b, b/a\} = \exp(|\log a - \log b|)$$

and in general, R satisfies a multiplicative triangle inequality:

$$R(A, C) \leqslant R(A, B)R(B, C).$$

The properties we need here are

$$R(A, B) \geqslant 1, \quad \text{and} \quad R(A, B) = 1 \Leftrightarrow A = B \tag{3.2}$$

and

$$R(A, B)^{-1}A \leqslant B \leqslant R(A, B)A, \tag{3.3}$$

which implies the norm bound

$$\|A - B\| \leqslant (R(A, B) - 1)\|A\|. \tag{3.4}$$

Here is our inductive definition of the geometric mean of $k > 2$ positive definite matrices, which will be extended to positive semidefinite matrices later. Suppose we have defined the geometric mean $G(X_1, \ldots, X_k)$ of k positive definite matrices $X_1, \ldots, X_k$. Consider the transformation on $(k + 1)$-tuples of positive definite matrices $A = (A_1, \ldots, A_{k+1})$ by

$$T(A) \equiv (G((A_i)_{i\neq 1}), G((A_i)_{i\neq 2}), \ldots, G((A_i)_{i\neq k+1})). \tag{3.5}$$

Here T should depend on k and may be better denoted by T_{k+1}. We drop the subscript $k+1$ for simplicity, and it is usually clear from the context.

Definition 3.1. (1) Define $G(A_1, A_2) = A_1\#A_2$—the usual geometric mean.

(2) Suppose we have defined the geometric mean $G(X_1, \ldots, X_k)$ of k positive definite matrices $X_1, \ldots, X_k$. We define the sequence $\{T^r(A)\}_{r=1}^{\infty}$. The limit of this sequence exists and has the form $(\tilde{A}, \ldots, \tilde{A})$. We define $G(A_1, \ldots, A_{k+1})$ to be $\tilde{A}$.

Sometimes it is useful to think of this iteration in terms of the components of the iterates:

$$A^{(1)} = (A_1, \ldots, A_{k+1}), \quad A^{(r+1)} = T(A^{(r)}),\ \ r = 1, 2, \ldots$$

To establish the validity of this definition we must show that the limit does indeed exist and that it has the asserted form. We do this in the next theorem.

Theorem 3.2. *Let* $A_1, \ldots, A_k$ *be positive definite. The sequences* $\{(A_1^{(r)}, \ldots, A_{k+1}^{(r)})\}_{r=1}^{\infty}$ *defined in Definition* 3.1 *do indeed converge to limits of the form* $(\tilde{A}, \ldots, \tilde{A})$, *and the geometric means defined above satisfy properties* P1–P9, *and*

$$R(G(A_1, \ldots, A_k), G(B_1, \ldots, B_k)) \leqslant \left\{\prod_{i=1}^{k} R(A_i, B_i)\right\}^{1/k}, \quad k = 2, 3, \ldots \tag{3.6}$$

Note:

- The continuity of G on the set of k-tuples of positive definite matrices follows from (3.6).
- The right side of (3.6) can be viewed as a measure of the distance between $(A_1, \ldots, A_k)$ and $(B_1, \ldots, B_k)$ in the multiplicative sense, i.e., the deviation of
$$(A_1B_1^{-1}, \ldots, A_kB_k^{-1}) \quad \text{from } (I, \ldots, I).$$
- In fact, (3.6) follows from the special case: If for some $i \in \{1, \ldots, k\}$, we have $A_j = B_j$ for $j \neq i$, then
$$R(G(A_1, \ldots, A_k), G(B_1, \ldots, B_k)) \leqslant R(A_i, B_i)^{1/k}, \quad k = 2, 3, \ldots$$

Proof. We use induction. For $k = 2$ we know that $A\#B$ satisfies properties P1–P9. We establish (3.6) when $k = 2$ with two proofs. The first one uses D4, and the second one uses some of the properties P1–P9. Different readers may have different preferences for the two proofs.

Proof 1. Using $A\#B = A^{1/2}UB^{1/2}$ where U is any unitary that makes the right-hand side positive definite, we have

$$\begin{aligned}
\rho(G(A_1, A_2)G(B_1, B_2)^{-1}) &= \rho(A_1^{1/2}UA_2^{1/2}B_2^{-1/2}V^*B_1^{-1/2}) \\
&= \rho(B_1^{-1/2}A_1^{1/2}UA_2^{1/2}B_2^{-1/2}V^*) \\
&\leqslant \left\|B_1^{-1/2}A_1^{1/2}UA_2^{1/2}B_2^{-1/2}V^*\right\| \\
&\leqslant \left\|B_1^{-1/2}A_1^{1/2}U\right\|\left\|A_2^{1/2}B_2^{-1/2}V^*\right\| \\
&= \left\|B_1^{-1/2}A_1^{1/2}\right\|\left\|A_2^{1/2}B_2^{-1/2}\right\| \\
&= \{\rho(A_1B_1^{-1})\rho(A_2B_2^{-1})\}^{1/2} \\
&\leqslant \{R(A_1, B_1)R(A_2, B_2)\}^{1/2}. \qquad \square
\end{aligned}$$

Proof 2. For any positive definite A_i, and B_i $(i = 1, 2)$ we have

$$B_i \leqslant \rho(A_i^{-1}B_i)A_i.$$

so by monotonicity and homogeneity

$$G(B_1, B_2) \leqslant \sqrt{\rho(A_1^{-1}B_1)\rho^{-1}(A_2^{-1}B_2)}G(A_1, A_2).$$

Thus

$$\rho(G(A_1, A_2)^{-1}G(B_1, B_2)) \leqslant \sqrt{\rho(A_1^{-1}B_1)\rho^{-1}(A_2^{-1}B_2)}. \qquad \square$$

Now, using Proof 1 or Proof 2, we can show

$$\rho(G(A_1, A_2)^{-1}G(B_1, B_2)) \leqslant \{R(A_1, B_1)R(A_2, B_2)\}^{1/2}.$$

As a result,

$$R(G(A_1, A_2), G(B_1, B_2)) \leqslant \{R(A_1, B_1)R(A_2, B_2)\}^{1/2}. \tag{3.7}$$

Next, suppose that $G(X_1, \dots, X_k)$ is defined and satisfies properties P1–P9, and (3.6). We show that the sequence $\{T^r(A)\}_{r=1}^{\infty}$ in the proposed construction of $G(A_1, \dots, A_{k+1})$ is convergent. By the special case of (3.6), we see that for each $r \geqslant 1$, we have

$$R(A_p^{(r+1)}, A_q^{(r+1)}) \leqslant R(A_p^{(r)}, A_q^{(r)})^{1/k}$$

for all $(p, q) \in \mathscr{S} = \{(1, 2), \dots, (k, k + 1), (k + 1, 1)\}$. So,

$$1 \leqslant \prod_{(p,q)\in\mathscr{S}} R(A_p^{(r+1)}, A_q^{(r+1)}) \leqslant \prod_{(p,q)\in\mathscr{S}} R(A_p^{(r)}, A_q^{(r)})^{1/k}. \tag{3.8}$$

Again, we can use two different arguments to arrive at our conclusion.

Argument 1. Now, by the induction assumption, we have G.M. $\leqslant$ A.M. for k matrices, and hence

$$A_j^{(r+1)} \leqslant \frac{1}{k}\sum_{i\neq j} A_i^{(r)}, \quad j = 1, \ldots, k+1.$$

Thus,

$$\sum_{i=1}^{k+1} A_i^{(r+1)} \leqslant \sum_{i=1}^{k+1} A_i^{(r)} \leqslant \sum_{i=1}^{k+1} A_i. \tag{3.9}$$

So, the sequence $\{(A_1^{(r)}, \ldots, A_{k+1}^{(r)})\}_{r=1}^{\infty}$ is bounded, and there must be a convergent subsequence, say, converging to $(\tilde{A}_1, \ldots, \tilde{A}_{k+1})$. By (3.8) and (3.2), we have

$$\prod_{(p,q)\in\mathscr{S}} R(\tilde{A}_p, \tilde{A}_q) = 1$$

and thus $\tilde{A}_1 = \cdots = \tilde{A}_{k+1}$, i.e., the limit of the subsequence has the form $(\tilde{A}, \ldots, \tilde{A})$. Suppose that there is another convergent subsequence converging to $(\tilde{B}, \ldots, \tilde{B})$. By (3.9), we have $\tilde{A} \geqslant \tilde{B}$ and $\tilde{B} \geqslant \tilde{A}$, i.e., $\tilde{A} = \tilde{B}$. Thus, the bounded sequence $\{(A_1^{(r)}, \ldots, A_{k+1}^{(r)})\}_{r=1}^{\infty}$ has only one limit point; so it is convergent.

Argument 2. Let $R_r = \prod_{(p,q)\in\mathscr{S}} R(A_p^{(r)}, A_q^{(r)})$. Then (3.8) is equivalent to

$$1 \leqslant R_{r+1} \leqslant (R_r)^{1/k}. \tag{3.10}$$

Take $i \neq j$ (without loss of generality, $i > j$). The multiplicative triangle inequality for R, and the fact that $R(X, Y) \geqslant 1$ for any X, Y gives us

$$R(A_j^{(r)}, A_i^{(r)}) \leqslant \prod_{k=j}^{i-1} R(A_k^{(r)}, A_{k+1}^{(r)}) \leqslant \prod_{(p,q)\in\mathscr{S}} R(A_p^{(r)}, A_q^{(r)}) = R_r. \tag{3.11}$$

We will show that the sequence $A_i^{(r)}$ is Cauchy to establish its convergence. To do this we bound $R(A_i^{(r+1)}, A_i^{(r)})$, and then convert it to a norm-wise bound via (3.4). Using (3.11) and (3.10) we have

$$\begin{aligned}
R(A_i^{(r+1)}, A_i^{(r)}) &= R(G((A_j^{(r)})_{j\neq i}), A_i^{(r)}) \\
&= R(G((A_j^{(r)})_{j\neq i}), G(A_i^{(r)}, \ldots, A_i^{(r)})) \\
&\leqslant \prod_{j\neq i} R(A_j^{(r)}, A_i^{(r)})^{1/k} \\
&\leqslant \prod_{j\neq i} R_r^{1/k} \\
&= R_r \\
&\leqslant R_{r-1}^{1/k} \\
&\;\;\vdots \\
&\leqslant R_1^{1/k^{r-1}}.
\end{aligned}$$

Let $R_1 = 1 + \alpha$. Then $R_1^{1/k^{r-1}} \leqslant 1 + \alpha/k^{r-1}$. So by (3.4) we have

$$\|A_i^{(r+1)} - A_i^{(r)}\| \leqslant (R_1^{1/k^{r-1}} - 1)M \leqslant \frac{1}{k^{r-1}}\alpha M,$$

where $M = \max\{\|A_j\| : j = 1, \dots, k+1\}$. Thus

$$\sum_{r=1}^{\infty} \|A_i^{(r+1)} - A_i^{(r)}\| \leqslant \sum_{r=1}^{\infty} \frac{1}{k^{r-1}}\alpha M < \infty.$$

That is, $\{A_i^{(r)}\}$ is a Cauchy sequence, and hence is convergent.

Now, we show that the newly defined $G(A_1, \dots, A_{k+1})$ satisfies property (3.6). To this end, take any positive definite matrices $A_1, \dots, A_{k+1}$ and $B_1, \dots, B_{k+1}$ and consider the sequences

$$\{(A_1^{(r)}, \dots, A_{k+1}^{(r)})\}_{r=1}^{\infty} \quad \text{and} \quad \{(B_1^{(r)}, \dots, B_{k+1}^{(r)})\}_{r=1}^{\infty}.$$

Then for any $r \geqslant 1$ and $j \in \{1, \dots, k+1\}$,

$$\begin{aligned} R(A_j^{(r+1)}, B_j^{(r+1)}) &= R(G((A_i^{(r)})_{i \neq j}), G((B_i^{(r)})_{i \neq j})) \\ &\leqslant \left\{ \prod_{i \neq j} R(A_i^{(r)}, B_i^{(r)}) \right\}^{1/k}. \end{aligned}$$

So,

$$\prod_{j=1}^{k+1} R(A_j^{(r+1)}, B_j^{(r+1)}) \leqslant \prod_{j=1}^{k+1} \left(\prod_{i \neq j} R(A_i^{(r)}, B_i^{(r)}) \right)^{1/k} = \prod_{i=1}^{k+1} R(A_i^{(r)}, B_i^{(r)}).$$

At the limit $(\tilde{A}, \dots, \tilde{A})$ and $(\tilde{B}, \dots, \tilde{B})$, we have

$$R(\tilde{A}, \tilde{B})^{k+1} \leqslant \prod_{i=1}^{k+1} R(A_i, B_i).$$

On taking $(k+1)$th roots we have the bound in (3.6).

Finally, consider properties P1–P9. These properties can be easily proved by induction and the fact that they are known to be true for $k = 2$. To illustrate that we prove

P3: For $k \geqslant 2$ we have $G(A_1, \dots, A_k) = G(A_{i_1}, \dots, A_{i_k})$ for any permutation $(i_1, \dots, i_k)$ of $(1, \dots, k)$.

We know that the result is true for $k = 2$. Now let us assume it is true for k and prove it for $k+1$. Let $(i_1, \dots, i_{k+1})$ be any permutation of $(1, \dots, k+1)$. Let $B_j = A_{i_j}$, $j = 1, \dots, k+1$. We will prove by induction that $B_j^{(r)} = A_{i_j}^{(r)}$ for

$j = 1, \ldots, k+1$ and $r = 2, 3, \ldots$. The result is true for $r = 1$ by assumption. Now assume the result for some $r \geqslant 1$ and prove it for $r + 1$.

$$\begin{aligned} B_j^{(r+1)} &= G((B_l^{(r)})_{l \neq j}) \\ &= G((A_{i_l}^{(r)})_{l \neq j}) \\ &= G((A_m^{(r)})_{m \neq i_j}) \\ &= A_{i_j}^{(r+1)}. \end{aligned}$$

Now that we have shown that $B_j^{(r)} = A_{i_j}^{(r)}$ for $j = 1, \ldots, k+1$ and $r = 2, 3, \ldots$, it follows that

$$(\tilde{B}, \ldots, \tilde{B}) = \lim_{r \to \infty} (B_1^{(r)}, \ldots, B_{k+1}^{(r)}) = \lim_{r \to \infty} (A_{i_1}^{(r)}, \ldots, A_{i_{k+1}}^{(r)}) = (\tilde{A}, \ldots, \tilde{A}).$$

Thus

$$G(A_{i_1}, \ldots, A_{i_{k+1}}) = \tilde{B} = \tilde{A} = G(A_1, \ldots, A_{k+1})$$

as desired. □

Since $G(A_1, \ldots, A_k)$ is order preserving, it also preserves positive definiteness. In fact, if $A_1, \ldots, A_k$ are positive definite and $\lambda_{\min}(A_i)I \leqslant A_i \leqslant \lambda_{\max}(A_i)I$ for $i = 1, \ldots, k$, then

$$\left(\prod_{i=1}^{k} \lambda_{\min}(A_i)\right)^{1/k} I \leqslant G(A_1, \ldots, A_k) \leqslant \left(\prod_{i=1}^{k} \lambda_{\max}(A_i)\right)^{1/k} I.$$

Now extend the definition of the geometric mean to the case of positive semidefinite matrices according to the standard procedure mentioned in Section 1. Then the extended geometric mean satisfies P1–P10 as well as P6′.

Theorem 3.3. *For any positive semidefinite matrices* $A_1, \ldots, A_k$

$$\operatorname{ran}(G(A_1, \ldots, A_k)) = \bigcap_{i=1}^{k} \operatorname{ran}(A_i), \quad k = 2, 3, \ldots \tag{3.12}$$

Proof. Take positive definite $A_{i,\epsilon}$ $(i = 1, 2, \ldots, k; \epsilon > 0)$ such that $A_{i,\epsilon} \downarrow A_i$ $(i = 1, 2, \ldots, k)$ as $\epsilon \downarrow 0$. Notice that by P10

$$G(A_{1,\epsilon}, \ldots, A_{k,\epsilon}) \geqslant k(A_{1,\epsilon}^{-1} + \ldots + A_{k,\epsilon}^{-1})^{-1}.$$

By definition the left-hand side converges to $G(A_1, \ldots, A_k)$ while it is known [1] that the right-hand side converges to the so-called *harmonic mean* $H(A_1, \ldots, A_k)$ of $A_1, \ldots, A_k$ and that

$$\operatorname{ran}(H(A_1, \ldots, A_k)) = \bigcap_{i=1}^{k} \operatorname{ran}(A_i).$$

Since the order relation for a pair of positive semidefinite matrices implies the inclusion relation of their ranges, we have

$$\operatorname{ran}(G(A_1, \dots, A_k)) \supset \bigcap_{i=1}^{k} \operatorname{ran}(A_i).$$

To prove the reverse inclusion, notice that by P6′ we have for any orthoprojection Q

$$G(QA_1Q, \dots, QA_kQ) \geqslant QG(A_1, \dots, A_k)Q.$$

By taking as Q the orthoprojection onto $\ker(A_1)$ and noting $QA_1Q = 0$, by P2 we can see

$$G(0, QA_2Q, \dots, QA_kQ) = 0 \geqslant QG(A_1, \dots, A_k)Q$$

which implies that

$$\ker(A_1) \subset \ker(G(A_1, \dots, A_k)).$$

By taking the orthogonal complements of both sides, we are led to the inclusion

$$\operatorname{ran}(A_1) \supset \operatorname{ran}(G(A_1, \dots, A_k)).$$

Since the same is true for each A_i in place of A_1, we can conclude

$$\bigcap_{i=1}^{k} \operatorname{ran}(A_i) \supset \operatorname{ran}(G(A_1, \dots, A_k)).$$

This completes the proof. □

The next result states that certain statements about $G(A_1, A_2)$ extend immediately to $G(A_1, \dots, A_k)$ for $k \geqslant 3$. Denote by P_r the set of $r \times r$ positive semidefinite matrices.

Theorem 3.4. *Let $\phi : P_n \to P_m$ be monotone, continuous from above, and continuous in the interior of P_n. Suppose*

$$G(\phi(X), \phi(Y)) - \phi(G(X, Y))$$

is positive semidefinite (respectively, negative semidefinite or zero) for any $X, Y \in P_n$. Then so is

$$G(\phi(A)) - \phi(G(A)) \tag{3.13}$$

for any $A = (A_1, \dots, A_k) \in P_n^k$ and any $k \geqslant 2$, where $\phi(A) = (\phi(A_1), \dots, \phi(A_k))$.

Proof. Our proof is by induction on k. Assume that we have the result for $k \geqslant 2$ and we wish to prove it for $k + 1$. Then for any $A = (A_1, \dots, A_{k+1}) \in P_n^{k+1}$ and $\varepsilon > 0$, let $A_\varepsilon = (A_1 + \varepsilon I, \dots, A_{k+1} + \varepsilon I)$. By the induction assumption,

$$
\begin{aligned}
T(\phi(A_\varepsilon)) &= T(\phi(A_1+\varepsilon I),\dots,\phi(A_{k+1}+\varepsilon I))\\
&= (G((\phi(A_i+\varepsilon I)_{i\neq 1}),\dots,G((\phi(A_i+\varepsilon I)_{i\neq k+1})))\\
&\geqslant (\phi(G((A_i+\varepsilon I)_{i\neq 1})),\dots,\phi((G(A_i+\varepsilon I)_{i\neq k+1})))\\
&= \phi(T(A_\varepsilon)).
\end{aligned}
$$

Iterating this we have

$$T^r(\phi(A_\varepsilon)) \geqslant \phi(T^r(A_\varepsilon)), \quad r=1,2,\dots$$

For any $\delta>0$, we have $T^r(\phi(A_\epsilon)+\delta(I,\dots,I)) \geqslant T^r(\phi(A_\epsilon))$. So,

$$T^r(\phi(A_\epsilon)+\delta(I,\dots,I)) \geqslant \phi(T^r(A_\varepsilon)), \quad r=1,2,\dots \tag{3.14}$$

Letting $r\to\infty$, we have $T^r(\phi(A_\epsilon)+\delta(I,\dots,I)) \to G(\phi(A_\epsilon)+\delta(I,\dots,I))$. Note that each coordinate in $T^r(A_\varepsilon)$ is larger than or equal to εI, and hence belongs to the interior of P_n. By continuity of ϕ on the interior of P_n, we see that the right side of (3.14) converges to $\phi(G(A_\varepsilon))$ as $r\to\infty$. Hence, $G(\phi(A_\epsilon)+\delta(I,\dots,I)) \geqslant \phi(G(A_\varepsilon))$, and

$$G(\phi(A_\epsilon)) = \lim_{\delta\downarrow 0} G(\phi(A_\epsilon)+\delta(I,\dots,I)) \geqslant \phi(G(A_\epsilon)).$$

Now, by the monotonicity of ϕ and G, we conclude that $G(\phi(A)) \geqslant \phi(G(A))$. $\square$

There are several inequalities one can derive from this result.

Let Φ be a positive linear map such that $\Phi(I)$ is positive definite. Clearly Φ is monotone, continuous from above (and continuous on the set of positive definite matrices just as mentioned for the geometric mean in Section 1). Then it is known that

$$\begin{pmatrix} X & Z \\ Z^* & Y \end{pmatrix} \geqslant 0, \quad Z=Z^* \Rightarrow \begin{pmatrix} \Phi(X) & \Phi(Z) \\ \Phi(Z^*) & \Phi(Y) \end{pmatrix} \geqslant 0$$

(see, e.g., [3, Corollary 4.4(ii)]). Note that the assertion $Z=Z^*$ is essential. So now, by definition D2, it follows that $\Phi(G(X,Y)) \leqslant G(\Phi(X),\Phi(Y))$. Thus by Theorem 3.4,

$$\Phi(G(A)) \leqslant G(\Phi(A)) \tag{3.15}$$

for any $A=(A_1,\dots,A_k)\in P_n^k$ with $k\geqslant 2$.

If we take

$$\phi(X) = \prod_{i=1}^r \lambda_i(X),$$

where λ_i denotes the ith largest eigenvalue, then we obtain the fact that for any $p\times p$ positive definite matrices $A_1,\dots,A_k$ and any $1\leqslant r\leqslant p$

$$\prod_{i=1}^r \lambda_i(G(A_1,\dots,A_k)) \leqslant \prod_{i=1}^r \left(\prod_{l=1}^k \lambda_i(A_l)\right)^{1/k}$$

and

$$\prod_{i=r}^{p} \lambda_i(G(A_1, \ldots, A_k)) \geqslant \prod_{i=r}^{p} \left(\prod_{l=1}^{k} \lambda_i(A_l) \right)^{1/k}.$$

We could partition a positive semidefinite matrix X as

$$X = \begin{pmatrix} X_{11} & X_{12} \\ X_{12}^* & X_{22} \end{pmatrix}$$

and take

$$\phi(X) = \begin{pmatrix} X_{11} - X_{12}X_{22}^{\dagger}X_{12}^* & 0 \\ 0 & 0 \end{pmatrix} \equiv \begin{pmatrix} S_X & 0 \\ 0 & 0 \end{pmatrix}.$$

That is, S_X denotes the Schur complement. It is known [8] that the generalized Schur complement can be characterized by

$$S_A = \max \left\{ X : A \geqslant \begin{pmatrix} X & 0 \\ 0 & 0 \end{pmatrix} \right\}. \tag{3.16}$$

This implies the monotonicity and the continuity from above of the map $A \mapsto S_A$. Since

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{12}^* & A_{22} \end{pmatrix} \geqslant \begin{pmatrix} S_A & 0 \\ 0 & 0 \end{pmatrix}, \quad \text{and} \quad B = \begin{pmatrix} B_{11} & B_{12} \\ B_{12}^* & B_{22} \end{pmatrix} \geqslant \begin{pmatrix} S_B & 0 \\ 0 & 0 \end{pmatrix}.$$

using monotonicity, we have

$$G(A, B) = A\#B \geqslant \begin{pmatrix} S_A & 0 \\ 0 & 0 \end{pmatrix} \# \begin{pmatrix} S_B & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} S_A\#S_B & 0 \\ 0 & 0 \end{pmatrix}. \tag{3.17}$$

Now, by the inequality (3.17) and the extremal representation (3.16), we have

$$S_{G(A,B)} \geqslant G(S_A, S_B).$$

Thus for any positive semidefinite $A_1, \ldots, A_k$ we have

$$S_{G(A_1,\ldots,A_k)} \geqslant G(S_{A_1}, \ldots, S_{A_k}).$$

Here let us pause to show that the Schur complement is useful for giving a representation of certain geometric means. For simplicity, with the orthoprojection

$$P = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}$$

let us abuse the notation $X_{11} \cdot P$ for the matrix

$$\begin{pmatrix} X_{11} & 0 \\ 0 & 0 \end{pmatrix}.$$

Let us show that for positive semidefinite A

$$A\#P = S_A^{1/2} \cdot P \tag{3.18}$$

Now, by D2 the geometric mean $G(A, P)$ is the solution of the extremal problem

$$\max\left\{X \geqslant 0 : \begin{pmatrix} A & X \\ X & P \end{pmatrix} \geqslant 0\right\}.$$

It is easy to see that positive definite X satisfies the inequality on the left-hand side if and only if $X = PXP$ and $X^2 \leqslant A$. Then by the extremal representation (3.16) of the Schur complement this implies $X^2 \leqslant S_A \cdot P$. Since the square-root function preserves the positive semidefinite order, we have

$$X \leqslant S_A^{1/2} \cdot P.$$

The matrix $X_0 \equiv S_A^{1/2} \cdot P$ satisfies the conditions $PX_0P = X_0$ and $X_0^2 \leqslant A$. This proves the asserted relation.

Notice that for positive definite A

$$S_A = (A^{-1})_{11}^{-1},$$

we can write

$$A\#P = (A^{-1})_{11}^{-1/2} \cdot P \qquad (\forall A > 0). \tag{3.19}$$

If we take $\phi(A) = C_q(A)$, be the qth multiplicative compound of an $n \times n$ matrix A $(1 \leqslant q \leqslant n)$, then D3 in Section 2 shows that $C_q(G(A_1, A_2)) = G(C_q(A_1), C_q(A_2))$; thus for any $A = (A_1, \ldots, A_k) \in P_n^k$ with $k \geqslant 2$ we have

$$C_q(G(A)) = G(C_q(A)).$$

Recall the qth additive compound Δ_q is defined by

$$\Delta_q(A) = \lim_{t \to 0} \frac{C_q(A + tI) - C_q(A)}{t}.$$

Let

$$J = \begin{pmatrix} I & I \\ I & I \end{pmatrix} \geqslant 0, \quad \text{and} \quad K = \begin{pmatrix} A & G(A, B) \\ G(A, B) & B \end{pmatrix}.$$

Since the multiplicative compound preserves the positive semidefinite order we have

$$W \equiv \lim_{t \to 0} \frac{C_q(K + tJ) - C_q(K)}{t} \geqslant 0.$$

One can check that

$$X \equiv \begin{pmatrix} \Delta_q(A) & \Delta_q(G(A, B)) \\ \Delta_q(G(A, B)) & \Delta_q(B) \end{pmatrix}$$

is a principal submatrix of the positive semidefinite matrix W, and so X is itself positive semidefinite. Thus,

$$G(\Delta_q(A), \Delta_q(B)) \geqslant \Delta_q(G(A, B)).$$

So taking $\phi = \Delta_q$ we have

$$G(\Delta_q(A)) \geqslant \Delta_q(G(A))$$

for any $A = (A_1, \ldots, A_k) \in P_n^k$ with $k \geqslant 2$.

To conclude this section, we observe that our geometric mean satisfies the following functional characterization.

Proposition 3.5. *The function G in Definition* 3.1 *is the only family of functions* $f_k : P_n^k \to P_n$, $k = 2, 3, \ldots$ *that satisfies*

(1) $f_2(A, B) = A\#B$.
(2) f_k *maps any* k*-tuples of positive semidefinite matrices to a positive semidefinite matrix and it is monotone and continuous from above*.
(3) f_k *maps any* k*-tuples of positive definite matrices to a positive definite matrix and it is continuous*.
(4) $f_k((A_i)_{i=1}^k) = f_k(f_{k-1}((A_i)_{i\neq 1}), \ldots, f_{k-1}((A_i)_{i\neq k}))$ *for* $k = 3, \ldots, n$.

This can be viewed as a functional characterization of G. Unfortunately, the fourth condition, which certainly is desirable, does not seem to be essential for a geometric mean.

One may wonder whether the properties P1–P9 are sufficient to characterize the geometric mean of more than two matrices. They are not sufficient, at least in the case of 2×2 matrices, as we show in Section 6.

We note that Dukes and Choi have proposed a geometric mean in the case $k = 3$ in unpublished notes [4]. Their mean is the same as ours, but their convergence proof is very different, not entirely clear, and appears to apply only to the case $k = 3$.

4. Other definitions of geometric means

In this section we show that extensions of some scalar definitions of the geometric mean and the definitions of the geometric mean of more than two positive definite matrices in the literature fail to satisfy at least one of the properties P1–P9, and that some even fail to satisfy one of the minimal properties P1–P6.

First let us see whether any of definitions D1–D5 of $G(A, B)$ in Section 2 extend easily to three matrices. Since three of more positive definite matrices may not be simultaneously diagonalizable by invertible congruence, it is not possible to use D1 for extension. It is not clear how to extend the definitions D2 and D3, but definition D4 suggests that we define the geometric mean $G_{uv}(A, B, C)$ to be $A^{1/3}UB^{1/3}VC^{1/3}$ where U and V to be unitary such that $A^{1/3}UB^{1/3}VC^{1/3}$ is positive definite. However, $A^{1/3}UB^{1/3}VC^{1/3} > 0$ depends on the choice of U, and V. This is most easily seen when A, B, C are all diagonal, and $(U, V) = (P, P^*)$ where P is a permutation other than the identity.

The definition D5 generalizes to $k > 2$ very naturally, and satisfies many, but not all of the desired properties. We dedicate the next section to it.

Let us now consider some other potential geometric means that generalize the scalar (commutative matrix) case. One may define

$$G_{\exp}(A_1, \ldots, A_k) = \exp\left\{\frac{\log(A_1) + \cdots + \log(A_k)}{k}\right\}.$$

This definition satisfies many of the conditions, but, even in the case $k = 2$, it is not monotone—because the exponential is not monotone on the space of Hermitian matrices, that is, $X \geqslant Y \not\Rightarrow e^X \geqslant e^Y$.

There are Hermitian matrices $X \geqslant Y$ such that $\exp(X) \ngeqslant \exp(Y)$.[2] Let

$$X_1 = Y_1 = Y, \quad X_2 = X - Y, \quad \text{and} \quad Y_2 = 0.$$

Then $X_1 \geqslant Y_1$ and $X_2 \geqslant Y_2$. Let $A_i = \exp(2X_i)$ and $B_i = \exp(2Y_i)$, for $i = 1, 2$. Then, because $2X_i$ and $2Y_i$ commute and the exponential is monotone on $\mathbb{R}$, we have $A_i \geqslant B_i$, for $i = 1, 2$. However,

$$\exp\left\{\frac{\log(A_1) + \log(A_2)}{2}\right\} = \exp(X) \ngeqslant \exp(Y) = \exp\left\{\frac{\log(B_1) + \log(B_2)}{2}\right\}.$$

One may try to define the geometric mean recursively in terms of # by

$$G_{\mathrm{rec}}(A, B, C) = (A^{4/3} \# B^{4/3}) \# C^{2/3}.$$

The right-hand side appears not be symmetric in A, B, and C and indeed it is not. Here is an example. Let us consider 2×2 matrices and let

$$P = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

Recall that from (3.19) we have

$$A \# P = (A^{-1})_{11}^{-1/2} \cdot P \qquad \forall\, A > 0.$$

Now, take $B = I$ and $C = P = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$. Then

---

[2] Consider

$$X \equiv 2I + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \geqslant \begin{pmatrix} 3/2 & 0 \\ 0 & 0 \end{pmatrix} \equiv Y.$$

Then

$$\exp(X) = e^2 \begin{pmatrix} \frac{e+e^{-1}}{2} & \frac{e-e^{-1}}{2} \\ \frac{e-e^{-1}}{2} & \frac{e+e^{-1}}{2} \end{pmatrix}, \quad \text{while} \quad \exp(Y) = \begin{pmatrix} e^{3/2} & 0 \\ 0 & 1 \end{pmatrix}.$$

Taking $x = [1, -1]^{\mathrm{T}}$, we have

$$x^{\mathrm{T}}(\exp(X) - \exp(Y))x = 2e^2e^{-1} - e^{3/2} - 1 = -0.045\ldots$$

Thus $\exp(X) \ngeqslant \exp(Y)$.

$$\begin{aligned} G_{\mathrm{rec}}(A, B, C) &= G_{\mathrm{rec}}(A, I, P) \\ &= (A^{4/3} \# I^{4/3}) \# P^{2/3} \\ &= (A^{4/3} \# I) \# P \\ &= A^{2/3} \# P \\ &= (A^{-2/3})_{11}^{-1/2} \cdot P. \end{aligned}$$

A similar calculation yields

$$G_{\mathrm{rec}}(A, C, B) = (A^{-4/3})_{11}^{-1/4} \cdot P.$$

So $G_{\mathrm{rec}}(A, B, C) = G_{\mathrm{rec}}(A, C, B)$ if and only if $(A^{-2/3})_{11}^{1/2} = (A^{-4/3})_{11}^{1/4}$, but this is not generally true. Here is an example:

$$A^{-2/3} = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}.$$

Then $(A^{-2/3})_{11}^{1/2} = \sqrt{2}$ while $(A^{-4/3})_{11}^{1/4} = \sqrt[4]{5}$.

Another idea that has been used in the scalar case to prove the arithmetic–geometric mean inequality is to define

$$G_{4\mathrm{rec}}(A, B, C, D) \equiv (A \# B) \# (C \# D)$$

and then define G_{34} to be the unique positive definite solution X to

$$G_{4\mathrm{rec}}(A, B, C, X) = X.$$

This fails because $G_{4\mathrm{rec}}$ itself is not symmetric in its arguments. Take 2×2 positive definite matrices A and B, and P as above, then

$$\begin{aligned} G_{4\mathrm{rec}}(A, B, P, P) &= (A \# B) \# (P \# P) = (A \# B) \# P \\ &= ((A \# B)^{-1})_{11}^{-1/2} \cdot P = (A^{-1} \# B^{-1})_{11}^{-1/2} \cdot P \end{aligned}$$

while

$$\begin{aligned} G_{4\mathrm{rec}}(A, P, B, P) &= (A \# P) \# (B \# P) \\ &= (A^{-1})_{11}^{-1/2} \cdot P \# (B^{-1})_{11}^{-1/2} \cdot P \\ &= ((A^{-1})_{11} (B^{-1})_{11})^{-1/4} \cdot P. \end{aligned}$$

Again these two are not the same since

$$(A^{-1} \# B^{-1})_{11} \leqslant ((A^{-1})_{11} (B^{-1})_{11})^{1/2}$$

and typically equality does not hold; for example, consider

$$A^{-1} = \begin{pmatrix} 4 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad B^{-1} = \begin{pmatrix} 8 & 2 \\ 2 & 2 \end{pmatrix}.$$

In this case $((A^{-1})_{11}(B^{-1})_{11})^{1/2} = 4\sqrt{2}$, but $(A^{-1} \# B^{-1})_{11} = 2(\sqrt{3} + 1)$ by Corollary 2.2.

There is a special case when $G_{4\text{rec}}$ is a permutationally invariant function of its arguments:

Proposition 4.1. *If A, B, C, D are positive definite $n \times n$ matrices such that $A\#B = C\#D \equiv G$. Then*

$$(A\#C)\#(B\#D) = (A\#D)\#(B\#C) = G. \tag{4.1}$$

Proof. First observe that if $A\#B = G$ then $B = GA^{-1}G$. Secondly, for any positive definite matrices X, Y

$$(X\#Y)\#(X^{-1}\#Y^{-1}) = (X\#Y)\#(X\#Y)^{-1} = I.$$

So now

$$\begin{aligned}
&G^{-1/2}[(A\#C)\#(B\#D)]G^{-1/2} \\
&\quad = G^{-1/2}[(A\#GD^{-1}G)\#(GA^{-1}G\#D)]G^{-1/2} \\
&\quad = (G^{-1/2}AG^{-1/2}\#G^{-1/2}GD^{-1}GG^{-1/2}) \\
&\qquad \#(G^{-1/2}GA^{-1}GG^{-1/2}\#G^{-1/2}DG^{-1/2}) \\
&\quad = (G^{-1/2}AG^{-1/2}\#G^{1/2}D^{-1}G^{1/2})\#(G^{1/2}A^{-1}G^{1/2}\#G^{-1/2}DG^{-1/2}) \\
&\quad = I.
\end{aligned}$$

For the last equality we have used the second observation with $X = G^{-1/2}AG^{-1/2}$ and $Y = G^{1/2}D^{-1}G^{1/2}$. $\square$

Trapp proposed two possible definitions for G_3 [9], and we will define them below. Anderson et al. extended them to k matrices with $k \geqslant 3$ in [2]. For two positive definite matrices, define $A : B = (A^{-1} + B^{-1})^{-1}$, which is half the harmonic mean of A and B. For three positive definite matrices A, B, C, define the symmetric means

$$\begin{aligned}
\Phi_1(A, B, C) &= (A + B + C)/3 \\
\Phi_2(A, B, C) &= [A : (B + C) + B : (C + A) + C : (A + B)]/2, \\
\Phi_3(A, B, C) &= 3(A^{-1} + B^{-1} + C^{-1})^{-1}
\end{aligned}$$

and define

$$\Phi_+(A, B, C) = (\Phi_1(A, B, C), \Phi_2(A, B, C), \Phi_3(A, B, C)).$$

Then the sequence $\{\Phi_+^r(A, B, C)\}_{r=1}^{\infty}$ will converge to a triple of matrices with all components equal. This common limit is called the upper AMT mean and is denoted by $G_{\text{amt}}^+(A, B, C)$.

Furthermore, define

$$G_{\text{amt}}^-(A, B, C) = G_{\text{amt}}^+(A^{-1}, B^{-1}, C^{-1})^{-1}$$

as the lower AMT mean, and $G_{\mathrm{amt}}(A, B, C) = G^{+}_{\mathrm{amt}}(A, B, C)\#G^{-}_{\mathrm{amt}}(A, B, C)$ as the AMT mean. Unfortunately, none of the three functions satisfies P2–joint homogeneity. Take

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}, \quad C = I_2.$$

Numerical computation shows that G^{+}_{amt}, G^{-}_{amt}, G_{amt} for (A, B, C) are:

$$\begin{pmatrix} 1.1587 & 0.5793 \\ 0.5793 & 1.1587 \end{pmatrix}, \quad \begin{pmatrix} 1.1507 & 0.5754 \\ 0.5754 & 1.1507 \end{pmatrix}, \quad \begin{pmatrix} 1.1547 & 0.5774 \\ 0.5774 & 1.1547 \end{pmatrix},$$

where as the corresponding means for $(A, B, 8C)$ are:

$$\begin{pmatrix} 2.3030 & 1.1393 \\ 1.1393 & 2.3030 \end{pmatrix}, \quad \begin{pmatrix} 2.2996 & 1.1376 \\ 1.1376 & 2.2996 \end{pmatrix}, \quad \begin{pmatrix} 2.3013 & 1.1385 \\ 1.1385 & 2.3013 \end{pmatrix}.$$

So,

$$G_3(A, B, 8I) \neq 2G_3(A, B, I)$$

for any of these three AMT means. Nevertheless, we will give some computational formulae related to them in the last section.

5. Kosaki mean

Kosaki [7] proposed a definition of the geometric mean of k positive definite matrices, which after later modification of the integral form by Kubo and Hiai, resulted in the following definition. Let

$$\alpha_j \geqslant 0 \ (j = 1, 2, \ldots, k) \quad \text{and} \quad \sum_{j=1}^{k} \alpha_j = 1.$$

For $A_j > 0$ $(j = 1, 2, \ldots, k)$ define

$$\begin{aligned} &(A_1, \ldots, A_k; \alpha_1, \ldots, \alpha_k) \\ &\quad \stackrel{\text{def}}{=} \frac{1}{\prod_{j=1}^{k} \Gamma(\alpha_j)} \int_{\Delta_k} \left\{ \sum_{j=1}^{k} \lambda_j A_j^{-1} \right\}^{-1} \left\{ \prod_{j=1}^{k} \lambda_j^{\alpha_j - 1} \right\} \mathrm{d}\lambda_1 \cdots \mathrm{d}\lambda_k, \end{aligned}$$

where

$$\Delta_k \stackrel{\text{def}}{=} \left\{ (\lambda_1, \ldots, \lambda_k); \lambda_k \geqslant 0 \ (k = 1, 2, \ldots, n), \ \sum_{j=1}^{k} \lambda_j = 1 \right\}.$$

The Kosaki mean on k positive definite matrices is

$$G_K^+(A_1, \dots, A_k) = (A_1, \dots, A_k; 1/k, \dots, 1/k) \tag{5.1}$$

$$= \frac{1}{\Gamma(1/k)^k} \int_{\Delta_k} \left\{ \sum_{j=1}^{k} \lambda_j A_j^{-1} \right\}^{-1} \left\{ \prod_{j=1}^{k} \lambda_j^{1/k-1} \right\} \mathrm{d}\lambda_1 \cdots \mathrm{d}\lambda_k. \tag{5.2}$$

The reason for denoting this mean by G_K^+ rather than G_K will become apparent later. An attractive feature of (5.2) is that if the A_i commute then we have a weighted geometric mean:

$$(A_1, \dots, A_k; \alpha_1, \dots, \alpha_k) = A_1^{\alpha_1} \cdots A_k^{\alpha_k}. \tag{5.3}$$

Let us show that in the case $k = 2$ this is indeed equal to #. We have the integral identity

$$\int_0^1 \frac{\lambda^{\alpha-1}(1-\lambda)^{\beta-1}}{\{\lambda a^{-1} + (1-\lambda)b^{-1}\}^{\alpha+\beta}} \, \mathrm{d}\lambda = \frac{\Gamma(\alpha) \cdot \Gamma(\beta)}{\Gamma(\alpha+\beta)} a^\alpha b^\beta.$$

With $\alpha = \beta = 1/2$ and $\Gamma(1/2)^2 = \pi$, so for any $C > 0$

$$C^{1/2} = \frac{1}{\pi} \int_0^1 \left\{ \lambda C^{-1} + (1-\lambda) \right\}^{-1} \left\{ \lambda^{-1/2} \cdot (1-\lambda)^{-1/2} \right\} \mathrm{d}\lambda.$$

Thus

$$\begin{aligned} A\#B &= A^{1/2}\left(A^{-1/2}BA^{-1/2}\right)^{1/2}A^{1/2} \\ &= \frac{1}{\pi} \int_0^1 \left\{ \lambda B^{-1} + (1-\lambda)A^{-1} \right\}^{-1} \left\{ \lambda^{-1/2} \cdot (1-\lambda)^{-1/2} \right\} \mathrm{d}\lambda. \\ &= G_K^+(A, B). \end{aligned}$$

It is easy to show that G_K^+ satisfies properties P1–P6. Some manipulation of integrals shows that G_K^+ satisfies P7 (homogeneity), at least in the case $k = 3$.

However, numerical computation shows that G_K^+ does not satisfy the determinant identity P9, nor self duality P8. Incidentally, when $n = 2$ and $k = 3$, G_K^+ does satisfy P9, but it still does not satisfy P8.

There is an easy way to modify G_K^+ so that the result is self dual. Define

$$G_K^-(A, B, C) \equiv G_K^+(A^{-1}, B^{-1}, C^{-1})^{-1}$$

and set

$$G_K(A, B, C) \equiv G_K^+(A, B, C) \# G_K^-(A, B, C).$$

The resulting geometric mean still satisfies conditions P1–P7, and by construction P8 also. However, numerical computation (below) shows that the new G_K still does not satisfy the determinant identity.

How did we compute $G_K(A, B, C)$? We computed $G_K^+(A, B, C)$ as follows. First, since G_K^+ satisfies congruence invariance

$$G_K^+(A, B, C) = C^{1/2} G_K^+(C^{-1/2}AC^{-1/2}, C^{-1/2}BC^{-1/2}, I)C^{1/2}.$$

We can reduce the double integral representation of G_K^+ to a single integral in the special case that $C = I$:

$$\begin{aligned} G_K^+(A, B, I) &= H(A, B) \\ &\equiv \frac{\Gamma(2/3)}{\Gamma(1/3)^2} \int_0^1 [u(1-u)]^{-2/3} \left(uA^{-1} + (1-u)B^{-1}\right)^{-2/3} \mathrm{d}u. \end{aligned}$$

The resulting integral can be numerically evaluated using Gauss–Jacobi quadrature with weight function $u^{-2/3}(1-u)^{-2/3}$. Golub and Welsch show how to compute the nodes and weights stably [5].

Do numerical errors invalidate our computations? We believe not, for the following reasons. Firstly we used well conditioned matrices, so there would be little error in computing A^{-1} and B^{-1}. It is known that for positive definite matrices and $0 \leqslant u \leqslant 1$, $(uA^{-1} + (1-u)B^{-1})^{-1}$ is at least as well conditioned as the worse conditioned of A and B, thus it too is well conditioned, and we can expect to make only very small errors in the required matrix computations.[3] What about the accuracy of the quadrature? The program delivered answers correct to about 15 digits when A and B were chosen to be scalars. For 3×3 matrices, as we increased p, the number of nodes used in quadrature, we noticed that the computed integrals appeared to converge, and in the end had a relative difference of about 10^{-14}—that is, they agreed to about 14 significant figures. We have not performed a careful error analysis because the above results suggest that our computations are more than accurate enough to demonstrate that G_K does not satisfy the determinant identity P9.

Here is a counter-example to the determinant identity: Let

$$A = \begin{pmatrix} 3 & 0 & 1 \\ 0 & 2 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \quad \text{and} \quad B = \begin{pmatrix} 2 & 0 & 1 \\ 0 & 3 & 1 \\ 1 & 1 & 1 \end{pmatrix}.$$

Both these matrices have integer inverses, and for any $u \in [0, 1]$, the linear combination $uA^{-1} + (1-u)B^{-1}$ has condition number less than 30. Then using Gauss quadrature with 40 nodes on MATLAB one gets

[3] It follows from [6, Cor 13.6] that if C is an $n \times n$ positive definite matrix, the X, the inverse computed using the Cholesky factorization and unit round off u (see [6, §2.2] for a precise definition) satisfies

$$\|X - C^{-1}\|_2 \leqslant 8n^{3.5}\kappa(C)\|C^{-1}\|_2 u + O(u^2).$$

In Matlab $u \approx 2 \times 10^{-16}$, so provided that $K(C)$, the condition number of C, and $\|C^{-1}\|$ are not too large, one can be sure that the computed C^{-1} is indeed close the true inverse.

$$G_K(A, B, I) = \begin{pmatrix} 1.71456842623973 & -0.02781758741820 & 0.61882347867050 \\ -0.02781758741820 & 1.71456842623973 & 0.61882347867050 \\ 0.61882347867050 & 0.61882347867050 & 0.79431436889448 \end{pmatrix}$$

which has determinant `0.99999964649328`, not 1. (Incidentally, when we used any number of nodes between 12 and 40, the computed determinant of $G_K(A, B, I)$ agreed to 14 decimal digits.)

Since G satisfies the determinantal identity, but G_K does not (by numerical computation), if follows that $G_K \neq G$. In the next section we restrict attention to 2×2 matrices. We show G_K does satisfy the determinant identity, but that nevertheless $G_K \neq G$, even in this special case.

6. Formulae for the 2 × 2 case

We would like to be able to define a geometric mean on $k > 2$ matrices without invoking a limiting process. However, even for some special 2×2 matrices, finding the closed form analytically does not not seem to be easy as shown in the example below.

In the subsequent discussion, we use the map

$$\Theta(X) \equiv \begin{pmatrix} x_{22} & -x_{12} \\ -x_{21} & x_{11} \end{pmatrix} \quad \text{for } X = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix}.$$

The map $\Theta(\cdot)$ is linear, involutive, and anti-multiplicative, i.e.,

$$\Theta(\alpha A + \beta B) = \alpha\Theta(A) + \beta\Theta(B), \quad \Theta^2(A) = A,$$
$$\Theta(AB) = \Theta(B) \cdot \Theta(A). \tag{6.1}$$

Important is the relation that

$$\det(\Theta(A)) = \det(A) \quad \text{and} \quad A^{-1} = \frac{\Theta(A)}{\det(A)} \quad \text{for invertible } A, \tag{6.2}$$

in particular,

$$A^{-1} = \Theta(A) \quad (\forall \det(A) = 1). \tag{6.3}$$

Further the following relation holds; for $A > 0$

$$\Theta(A^p) = \Theta(A)^p \quad (p \in \mathbb{R}), \text{ in particular } \Theta(A)^{-1} = \Theta(A^{-1}). \tag{6.4}$$

Example 6.1. If

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}, \quad \text{and} \quad C = I_2,$$

then numerical computations show that

$$G(A, B, C) = \frac{1}{\sqrt{3}} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix},$$

which is equal to $c(A + B + C)$ with $c > 0$ satisfying $\det c(A + B + C) = 1$.

To prove the result analytically, let $(A_0, B_0, C_0) = (A, B, C)$, and for $r \geqslant 1$

$$A_{r+1} \equiv B_r \# C_r, \quad B_{r+1} \equiv C_r \# A_r, \quad C_{r+1} \equiv A_r \# B_r.$$

We prove by induction that there are $\alpha_r, \beta_r \geqslant 0$ such that

$$\begin{aligned} A_r &= \alpha_r A + \beta_r B + \beta_r C, \\ B_r &= \beta_r A + \alpha_r B + \beta_r C, \\ C_r &= \beta_r A + \beta_r B + \alpha_r C. \end{aligned}$$

Clearly, $\alpha_0 = 1$ and $\beta_0 = 0$. Suppose that the relations are true for r. Since

$$\det(A_r) = \det(B_r) = \det(C_r) = 1,$$

we have, Proposition 2.1,

$$\begin{aligned} A_{r+1} &= \frac{1}{\sqrt{2 + \operatorname{tr}(\Theta(B_r) \cdot C_r)}}(B_r + C_r), \\ B_{r+1} &= \frac{1}{\sqrt{2 + \operatorname{tr}(\Theta(C_r) \cdot A_r)}}(C_r + A_r), \\ C_{r+1} &= \frac{1}{\sqrt{2 + \operatorname{tr}(\Theta(A_r) \cdot B_r)}}(A_r + B_r). \end{aligned}$$

Since

$$\operatorname{tr}(\Theta(A) \cdot A) = \operatorname{tr}(\Theta(B) \cdot B) = \operatorname{tr}(\Theta(C) \cdot C) = 2$$

and

$$\begin{aligned} \operatorname{tr}(\Theta(A) \cdot B) &= \operatorname{tr}(\Theta(A) \cdot C) = 3, \\ \operatorname{tr}(\Theta(B) \cdot A) &= \operatorname{tr}(\Theta(B) \cdot C) = 3, \\ \operatorname{tr}(\Theta(C) \cdot A) &= \operatorname{tr}(\Theta(C) \cdot B) = 3, \end{aligned}$$

by the induction assumption

$$\begin{aligned} \operatorname{tr}(\Theta(B_r) \cdot C_r) &= \operatorname{tr}\Big(\{\beta_r \Theta(A) + \alpha_r \Theta(B) + \beta_r \Theta(C)\}\{\beta_r A + \beta_r B + \alpha_r C\}\Big) \\ &= \beta_r(2\beta_r + 3\beta_r + 3\alpha_r) + \alpha_r(3\beta_r + 2\beta_r + 3\alpha_r) \\ &\quad + \beta_r(3\beta_r + 3\beta_r + 2\alpha_r) \\ &= 3\alpha_r^2 + 10\alpha_r\beta_r + 11\beta_r^2; \end{aligned}$$

similarly,

$$\operatorname{tr}(\Theta(C_r) \cdot A_r) = 3\alpha_r^2 + 10\alpha_r\beta_r + 11\beta_r^2$$

and

$$\mathrm{tr}(\Theta(A_r)\cdot B_r)=3\alpha_r^2+10\alpha_r\beta_r+11\beta_r^2,$$

Therefore we have

$$\mathrm{tr}(\Theta(B_r)\cdot C_r)=\mathrm{tr}(\Theta(C_r)\cdot A_r)=\mathrm{tr}(\Theta(A_r)\cdot B_r)\equiv\gamma_r.$$

Then by definition and the induction assumption

$$\begin{aligned}A_{r+1}=B_r\#C_r&=\frac{B_r+C_r}{\sqrt{2+\mathrm{tr}(\Theta(B_r)\cdot C_r)}}\\&=\frac{(2\beta_r)A+(\alpha_r+\beta_r)B+(\alpha_r+\beta_r)C}{\sqrt{2+\gamma_r}}\end{aligned}$$

and similarly

$$\begin{aligned}B_{r+1}=C_r\#A_r&=\frac{C_r+A_r}{\sqrt{2+\mathrm{tr}(\Theta(C_r)\cdot A_r)}}\\&=\frac{(\alpha_r+\beta_r)A+(2\beta_r)B+(\alpha_r+\beta_r)C}{\sqrt{2+\gamma_r}},\\C_{r+1}=A_r\#B_r&=\frac{A_r+B_r}{\sqrt{2+\mathrm{tr}(\Theta(A_r)\cdot B_r)}}\\&=\frac{(\alpha_r+\beta_r)A+(\alpha_r+\beta_r)B+(2\beta_r)C}{\sqrt{2+\gamma_r}}.\end{aligned}$$

Therefore with

$$\begin{aligned}\alpha_{r+1}&\equiv\frac{2\beta_r}{\sqrt{2+\gamma_r}}=\frac{2\beta_r}{\sqrt{2+3\alpha_r^2+10\alpha_r\beta_r+11\beta_r^2}},\\\beta_{r+1}&\equiv\frac{\alpha_r+\beta_r}{\sqrt{2+\gamma_r}}=\frac{\alpha_r+\beta_r}{\sqrt{2+3\alpha_r^2+10\alpha_r\beta_r+11\beta_r^2}}\end{aligned}$$

we have

$$\begin{aligned}A_{r+1}&=\alpha_{r+1}A+\beta_{r+1}B+\beta_{r+1}C,\\B_{r+1}&=\beta_{r+1}A+\alpha_{r+1}B+\beta_{r+1}C,\\C_{r+1}&=\beta_{r+1}A+\beta_{r+1}B+\alpha_{r+1}C.\end{aligned}$$

This completes the induction. Since A, B, C are linearly independent and

$$G(A,B,C)=\lim_{r\to\infty}A_r=\lim_{r\to\infty}B_r=\lim_{r\to\infty}C_r,$$

we can conclude that

$$\lim_{r\to\infty}\alpha_r=\lim_{r\to\infty}\beta_r\equiv\alpha$$

and

$$G(A,B,C)=\alpha(A+B+C).$$

Since $\det(G(A, B, C)) = 1$, the value α is determined by

$$\alpha^2 \det(A + B + C) = 1,$$

so that

$$\alpha = \frac{1}{\sqrt{12}} \quad \text{and} \quad G(A, B, C) = \frac{1}{\sqrt{3}} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}.$$

This completes the proof.

Next, we prove some formulae for the other geometric means on three 2×2 matrices that may be useful for future study.

Proposition 6.2. *If* $A, B, C > 0$ *are* 2×2 *and such that* $\det(A) = \det(B) = \det(C) = 1$, *then for the Kosaki mean the following holds*:

$$G_K^+(A, B, C) = \alpha A + \beta B + \gamma C,$$

where

$$\alpha \equiv \frac{1}{\Gamma(1/3)^3} \int_{\Delta_3} \frac{\lambda_1 \cdot (\lambda_1\lambda_2\lambda_3)^{-2/3}}{\det(\lambda_1 A + \lambda_2 B + \lambda_3 C)} \, \mathrm{d}\lambda_1 \, \mathrm{d}\lambda_2 \, \mathrm{d}\lambda_3,$$

$$\beta \equiv \frac{1}{\Gamma(1/3)^3} \int_{\Delta_3} \frac{\lambda_2 \cdot (\lambda_1\lambda_2\lambda_3)^{-2/3}}{\det(\lambda_1 A + \lambda_2 B + \lambda_3 C)} \, \mathrm{d}\lambda_1 \, \mathrm{d}\lambda_2 \, \mathrm{d}\lambda_3,$$

$$\gamma \equiv \frac{1}{\Gamma(1/3)^3} \int_{\Delta_3} \frac{\lambda_3 \cdot (\lambda_1\lambda_2\lambda_3)^{-2/3}}{\det(\lambda_1 A + \lambda_2 B + \lambda_3 C)} \, \mathrm{d}\lambda_1 \, \mathrm{d}\lambda_2 \, \mathrm{d}\lambda_3.$$

Moreover,

$$G_K^-(A, B, C) = \frac{G_K^+(A, B, C)}{\det(G_K^+(A, B, C))}$$

and

$$G_K(A, B, C) = \frac{G_K^+(A, B, C)}{\sqrt{\det(G_K^+(A, B, C))}}.$$

Proof. For simplicity, write

$$\sigma(\lambda_1, \lambda_2, \lambda_3) \equiv \frac{1}{\Gamma(1/3)^3} (\lambda_1\lambda_2\lambda_3)^{-2/3} \mathrm{d}\lambda_1 \mathrm{d}\lambda_2 \mathrm{d}\lambda_3.$$

Then

$$G_K^+(A, B, C) = \int_{\Delta_3} (\lambda_1 A^{-1} + \lambda_2 B^{-1} + \lambda_3 C^{-1})^{-1} \, \mathrm{d}\sigma(\lambda_1, \lambda_2, \lambda_3). \tag{6.5}$$

Since in the present case

$$A^{-1} = \Theta(A), \quad B^{-1} = \Theta(B), \quad C^{-1} = \Theta(C)$$

we have

$$G_K^+(A, B, C) = \int_{\Delta_3} \Theta(\lambda_1 A + \lambda_2 B + \lambda_3 C)^{-1}\, \mathrm{d}\sigma(\lambda_1, \lambda_2, \lambda_3) \times \int_{\Delta_3} \frac{\lambda_1 A + \lambda_2 B + \lambda_3 C}{\det(\lambda_1 A + \lambda_2 B + \lambda_3 C)}\, \mathrm{d}\sigma(\lambda_1, \lambda_2, \lambda_3).$$

Next

$$G_K^-(A, B, C) \equiv G_K^+(A^{-1}, B^{-1}, C^{-1})^{-1} = G_K^+(\Theta(A), \Theta(B), \Theta(C))^{-1} = \Theta(G_K^+(A, B, C))^{-1} = \frac{G_K^+(A, B, C)}{\det(G_K^+(A, B, C))}.$$

Finally

$$G_K(A, B, C) = G_K^+(A, B, C) \# G_K^-(A, B, C) = \frac{G_K^+(A, B, C)}{\sqrt{\det(G_K^+(A, B, C))}}.$$

This completes the proof. □

The formula for G_K given in Proposition 6.2 shows that G_K satisfies the determinant identity (P9) when A, B, C are 2×2 and have determinant 1. Since G_K can be shown to satisfy joint homogeneity (P2), it follows that G_K satisfies P9 for all $A, B, C > 0$ (assumed 2×2). Thus, both G_K and our new G satisfy conditions P1–P9, but they are not equal. Here is an example. Take

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}, \quad C = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Then numerical computation shows that

$$G(A, B, C) = \begin{pmatrix} 0.9319 & 0.6636 \\ 0.6636 & 1.5456 \end{pmatrix}, \quad G_K(A, B, C) = \begin{pmatrix} 0.9320 & 0.6628 \\ 0.6628 & 1.5444 \end{pmatrix}.$$

Finally, we give a closed formula for the AMT means of 2×2 positive definite matrices A, B, C each of which has determinant 1. Since these means are not jointly homogeneous this proposition does not yield a formula for general triplets of positive definite matrices.

Proposition 6.3. *Let* $A, B, C > 0$ *be* 2×2 *and such that* $\det(A) = \det(B) = \det(C) = 1$. *Then*

$$G_{\mathrm{amt}}^+(A, B, C) = \frac{1}{\det(\tilde{A})^{1/3}} \tilde{A}^{1/2} \cdot \left(\tilde{A}^{-1/2} \tilde{B} \tilde{A}^{-1/2}\right)^{1/3} \cdot \tilde{A}^{1/2},$$

where $\tilde{A}$, $\tilde{B}$ (*and* $\tilde{C}$) *are the matrices in the first step of the iterations*

$$\begin{aligned}\tilde{A} &\equiv \tfrac{1}{3}(A+B+C),\\ \tilde{B} &\equiv \tfrac{1}{2}\{A:(B+C)+B:(C+A)+C:(A+B)\},\\ \tilde{C} &\equiv 3(A:B:C).\end{aligned}$$

Moreover,

$$G^-_{\mathrm{amt}}(A,B,C)=\frac{G^+_{\mathrm{amt}}(A,B,C)}{\det(G^+_{\mathrm{amt}}(A,B,C))}$$

and

$$G_{\mathrm{amt}}(A,B,C)=\frac{G^+_{\mathrm{amt}}(A,B,C)}{\sqrt{\det(G^+_{\mathrm{amt}}(A,B,C))}}.$$

Proof. First, note that

$$\begin{aligned}\tilde{C} &= 3(A^{-1}+B^{-1}+C^{-1})^{-1}\\ &= 3\Big(\Theta(A)+\Theta(B)+\Theta(C)\Big)^{-1}\\ &= \frac{3}{\det(A+B+C)}(A+B+C) \;=\; \frac{1}{\det(\tilde{A})}\tilde{A}.\end{aligned}$$

Next, we show that if $C=\rho A$ with $\rho>0$, then

$$G^+_{\mathrm{amt}}(A,B,C)=\rho^{1/3}A^{1/2}\cdot(A^{-1/2}BA^{-1/2})^{1/3}\cdot A^{1/2}.$$

This is true because

$$G^+_{\mathrm{amt}}(A,B,C)=A^{1/2}\cdot G^+_{\mathrm{amt}}\Big(I,A^{-1/2}BA^{-1/2},\rho I\Big)\cdot A^{1/2}$$

and I, $A^{-1/2}BA^{-1/2}$, ρI are commuting, and thus

$$G^+_{\mathrm{amt}}\Big(I,A^{-1/2}BA^{-1/2},\rho I\Big)=\rho^{1/3}(A^{-1/2}BA^{-1/2})^{1/3}.$$

Combining the above observations, we get the formula for $G^+_{\mathrm{amt}}(A,B,C)$.

Let $(A_1,B_1)=(\tilde{A},\tilde{B})$. Then

$$G^+_{\mathrm{amt}}(A,B,C)=\frac{1}{\det(A_1)^{1/3}}A_1^{1/2}\Big(A_1^{-1/2}B_1A_1^{-1/2}\Big)^{1/3}A_1^{1/2}. \tag{6.6}$$

First notice that

$$\frac{A^{-1}+B^{-1}+C^{-1}}{3}=\Theta(A_1)$$

and

$$\begin{aligned}2B_1 = (A+B+C) &- A(A+B+C)^{-1}A\\ &-B(A+B+C)^{-1}B-C(A+B+C)^{-1}C.\end{aligned}$$

Replacing A, B, C by A^{-1}, B^{-1}, C^{-1}, by (6.4) we have

$$\begin{aligned}
&(A^{-1}+B^{-1}+C^{-1}) - A^{-1}(A^{-1}+B^{-1}+C^{-1})^{-1}A^{-1}\\
&\quad -B^{-1}(A^{-1}+B^{-1}+C^{-1})^{-1}B^{-1} - C^{-1}(A^{-1}+B^{-1}+C^{-1})^{-1}C^{-1}\\
&= \Theta(A+B+C) - \Theta(A)\Theta(A+B+C)^{-1}\Theta(A)\\
&\quad -\Theta(B)\Theta(A+B+C)^{-1}\Theta(B) - \Theta(C)\Theta(A+B+C)^{-1}\Theta(C)\\
&= 2\Theta(B_1).
\end{aligned}$$

Therefore by (6.6) and (6.4)

$$\begin{aligned}
&G^{+}_{\mathrm{amt}}(A^{-1}, B^{-1}, C^{-1})^{-1}\\
&\quad = \left\{\frac{1}{\det(\Theta(A_1))^{1/3}}\Theta(A_1)^{1/2}\Big(\Theta(A_1)^{-1/2}\Theta(B_1)\Theta(A_1)^{-1/2}\Big)^{1/3}\Theta(A_1)^{1/2}\right\}^{-1}\\
&\quad = \Theta(G^{+}_{\mathrm{amt}}(A, B, C))^{-1} = \frac{G^{+}_{\mathrm{amt}}(A, B, C)}{\det(G^{+}_{\mathrm{amt}}(A, B, C))};
\end{aligned}$$

hence

$$G^{-}_{\mathrm{amt}}(A, B, C) = \frac{G^{+}_{\mathrm{amt}}(A, B, C)}{\det(G^{+}_{\mathrm{amt}}(A, B, C))}$$

and

$$G_A(A, B, C) = \frac{G^{+}_{\mathrm{amt}}(A, B, C)}{\sqrt{\det(G^{+}_{\mathrm{amt}}(A, B, C))}}.$$

This completes the proof. □

As explained at the end of Section 2, by Proposition 6.3 one can write $G_{\mathrm{amt}}(A, B, C)$ in a form $\alpha A + \beta B + \gamma C$. But the explicit formulas for α, β, γ are quite complicated. For the matrices in Example 6.1 we can show

$$G_K(A, B, C) = G_{\mathrm{amt}}(A, B, C) = \frac{1}{\sqrt{3}}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} = G(A, B, C).$$

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